Generative chemistry: drug discovery with deep learning generative models

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Abstract

The de novo design of molecular structures using deep learning generative models introduces an encouraging solution to drug discovery in the face of the continuously increased cost of new drug development. From the generation of original texts, images, and videos, to the scratching of novel molecular structures the creativity of deep learning generative models exhibits the height machine intelligence can achieve. The purpose of this paper is to review the latest advances in generative chemistry which relies on generative modeling to expedite the drug discovery process. This review starts with a brief history of artificial intelligence in drug discovery to outline this emerging paradigm. Commonly used chemical databases, molecular representations, and tools in cheminformatics and machine learning are covered as the infrastructure for generative chemistry. The detailed discussions on utilizing cutting-edge generative architectures, including recurrent neural network, variational autoencoder, adversarial autoencoder, and generative adversarial network for compound generation are focused. Challenges and future perspectives follow.